Sensitivities and Variances for Fitted Parameters of Spheres

By

Christoph Witzgall and Marek Franaszek

Abstract

Experimental data have been gathered by applying 3D imaging systems, such as LIDAR/LADAR instruments, to spherical objects. This report provides a compilation of the statistical and analytical procedures to be used for an evaluation, to be reported separately, of two different methods of modeling objects, directional and orthogonal fitting, based on those data. Estimating the variances of fitted parameters directly from their sensitivities to data perturbations is proposed. Sensitivities are determined by implicit differentiation of error gradiens. Detailed descriptions of the directional and orthogonal fitting methods, as applied to spheres in a scanning environment, are set forth. In particular, the report furnishes closed-form expressions for those derivatives of the respective error functions which are needed for the calculation of the parameter sensitivities with respect the full set of control variables.

Key Words

3D imaging systems, directional fitting, least squares, LIDAR/LADAR, orthogonal distance fitting, parameter variance, parameter sensitivity, sphere, statistical modeling

1 Introduction

A frequent task is to determine the shape characteristics, size, position and pose of physical objects for purposes of identification, location, registration, and calibration of coordinate frames. Such tasks are needed, among others, for quality control in manufacturing, determination of "as-built" structures, construction automation and site monitoring, e.g., [1, 2].

A common approach to these tasks is to acquire 3D coordinates of data points considered to lie on the surface of targeted objects. 3D Imaging Systems, which include "line-of-sight" LIDAR/LADAR devices, are increasingly used for this purpose. The latter instruments, in particular, are capable of fast generation of large amounts of data points or "point clouds". They scan an object by emitting laser pulses and processing return signals in order to determine the distance traveled and thus determine the distance or "range" between the instrument and the point of impact -- presumably -- on the object. The device keeps track of the "bearings" such as azimuth and elevation angle, at which each particular signal was emitted. This process of data acquisition suggested the use in this work of polar/spherical ("angle-angle-range") coordinate systems for representing data points. Also, transformation to Cartesian coordinates will introduce correlation.

Once the point cloud corresponding to an object has been determined, a computational process is required to extract the desired features of the object from this data set. In typical applications, a mathematical "model" is specified, based on features characteristic for a class of objects. The model is "parameterized", that is, it is defined with the help of parameters that determine these characteristics. Choosing values for these parameters will result in the mathematical description of a surface to represent a "virtual object", which may then be compared to an image of the real object as provided by the point cloud. By adjusting the model parameters so that the virtual object moves into a location that optimizes the proximity of the object surface to points in the point cloud, desired characteristics such as location, pose, size and shape are found within the coordinate frame of the point cloud. This permits determining the geometric relationship between that object and other objects or features that are also represented in the point cloud frame. If this frame registers to an established ground-truth frame, then absolute measurements of location, pose and shape can be extracted.

Such approaches to the modeling of objects of interest within a point cloud may employ the powerful "Iterative Closest Point (ICP)" method [3], or the "Hough Transform", e.g. [4]. Present work focuses on the extensively used "Fitting" paradigm, which is based on minimizing a specified error function or on maximizing likelihood. The reader may want to consult texts on "Statistical Models" such as [5-7].

Of particular interest are two least-squares based approaches, "orthogonal" and "directional" fitting. Orthogonal fitting, also referred to as "Orthogonal Distance Regression (ODR)" [8, 9], or "Geometric Fitting" [10], is a commonly used and widely commercialized method. In particular, publications [10-19] discuss its application to the fitting of spheres or circles. The alternate approach, "directional fitting" has been proposed and discussed [20, 21] for data acquired by scanning from a single instrument position. Here, the orthogonal (closest Euclidean) distance to the virtual object has been replaced by the distance in the direction of the scan by which the data point had been acquired. While computational aspects dominate much of this research, our interest here is in statistical and metrological issues.

The thrust of this report is an approach to determining the sensitivities of fitted model parameters, in general, and for spherical models, in particular. The report is also preparatory to an experimental study of different fitting methods and their statistical evaluation [22]. At issue, in particular, is the estimation of derived variances for fitted sphere centers based on specified variances for range measurements. In Chapter 2, the general fitting paradigm, based on the concept of an error function, is described, along with the general computational formalism for calculating parameter sensitivities. These sensitivities will be used to estimate parameter variances. In dealing with spherical models, this approach is of necessity more general than the common nonlinear least squares approach based on linearization and homoscedacity. A comparative discussion of these statistical procedures will be provided in a separate report [23]. Chapters 3 and 4 are dedicated, respectively, to orthogonal and directional fitting of spheres in a scanning environment. Closed forms of the derivatives, needed for calculating sensitivities, are reported. The Appendix will feature detailed derivations of the reported formulas so as to enable verification.

2 The Fitting Paradigm

2.1 Error Function

Once a parameterized model has been selected, it is natural to ask for parameters that minimize the extent to which the point cloud deviates from the resulting virtual object. The hope is that such an – at least locally – optimal virtual object provides, within the coordinate frame of the data points, an accurate representation of the actual object. Fitting a 3D model of a sphere of a Cartesian center $C = [X, Y, Z]$ and known radius R may be accomplished by specifying an "error function"

$$E = E(X, Y, Z, d_1, \varphi_1, \theta_1, d_2, \varphi_2, \theta_2, ..., d_n, \varphi_n, \theta_n) \qquad (2.1.1)$$

where X, Y, Z denote the model parameters, and the variables $d_i, \varphi_i, \theta_i, i = 1,...,n,$ are coordinates of points $\boldsymbol{P}_i = [d_i \quad \varphi_i \quad \theta_i]$ to be measured. The following discussions, however, should not be construed as pertaining only to this special scenario, but rather as representative of full generality. In particular, the data may also be Cartesian, or not be coordinates, at all.

The choice of the error function should be such that it produces only nonnegative values. A minimum of zero should indicate a perfect fit. An error function E thus furnishes a model description.

Given an actual data set of measurements

$$\boldsymbol{P}_i^{(0)} = [d_i^{(0)} \quad \varphi_i^{(0)} \quad \theta_i^{(0)}],\ i = 1, ..., n,$$

the parameter values

$$X = X^{(0)}, Y = Y^{(0)}, Z = Z^{(0)}$$

are thus determined by minimizing the expression

$$E = E(X, Y, Z, d_1^{(0)}, \varphi_1^{(0)}, \theta_1^{(0)}, d_2^{(0)}, \varphi_2^{(0)}, \theta_2^{(0)}, ..., d_n^{(0)}, \varphi_n^{(0)}, \theta_n^{(0)})$$

for the variables X, Y, Z, given the coordinate values of the data points $\boldsymbol{P}_i$.

A common approach to constructing error functions is to assign an individual error

$$e_i = e_i(X, Y, Z, d_i, \varphi_i, \theta_i)$$

to each data point $\boldsymbol{P}_i = [d_i \quad \varphi_i \quad \theta_i]$, and to minimize the sum of squares

$$(2.1.2) \qquad E = \sum_{i=1}^{n} e_i^2 .$$

Both, the orthogonal and directional fitting method, mentioned in the Introduction, are based on the Nonlinear Least Squares (NLS) concept [17, 19]. In both cases, each data point $\boldsymbol{P}_i$ is assigned a "theoretical point" or "model point" $\hat{\boldsymbol{P}}_i$ located on the proposed virtual object. That theoretical point is seen as the desired "correct" point, and the Euclidean distance between the two points is considered the individual error

$$e_i = \left\| \hat{\boldsymbol{P}}_i - \boldsymbol{P}_i \right\|$$

of the data point with respect to the current location and shape specification of the virtual object.

In orthogonal fitting, the theoretical point $\hat{\boldsymbol{P}}_i$ is chosen as a point that lies on the virtual object and is closest to the data point $\boldsymbol{P}_i$ in terms of Euclidean distance. In the 3D imaging environment, however, the data point $\boldsymbol{P}_i$ is considered to lie on a particular "scan ray" or "line-of-sight", which emanates from the instrument position.
In directional fitting, if the scan ray intersects the virtual object, the intersection closest to the instrument is thus chosen as the theoretical point $\hat{\boldsymbol{P}}_i$ for the data point $\boldsymbol{P}_i$. What happens if the scan ray of a data point $\boldsymbol{P}_i$ does not intersect the current virtual object? It might be tempting to reject such an occurrence as unrealistic as the point cloud was generated from the real object. It should be kept in mind, however, that during the fitting process, the virtual object will, in general, not match the actual object. Indeed, establishing that match is the purpose of the fitting process. It is, therefore, necessary to extend the error definition to those date points whose scan rays miss the virtual object. The following generic principle for a continuous extension has been proposed in [21]. Here, the theoretical point $\hat{\boldsymbol{P}}_i$ is chosen as a point on the virtual object that is closest to the scan ray in terms of Euclidean distance.

2.2 Sensitivity

As we return to the general error function E (2.1.1), we examine a major aspect of analyzing the results of a fitting procedure. It concerns the "sensitivities" of the resulting parameters, namely, their marginal rates of change caused by perturbations of the data coordinates. Such sensitivities not only provide key information about a fitting process, they also play a role in the estimation of variances and covariances of the fitted parameters, as will be discussed in the subsequent section.

With each set of stipulated data values $d_i, \varphi_i, \theta_i,\ i, \ldots, n$, the error function E associates a set of minimizing parameters. We may thus consider the minimizing parameters as functions of these data variables

$$(2.2.1) \qquad X(d_1, \varphi_1, \theta_1, \ldots, d_n, \varphi_n, \theta_n)$$

$$Y(d_1,\varphi_1,\theta_1,\ldots,d_n,\varphi_n,\theta_n)$$
$$Z(d_1,\varphi_1,\theta_1,\ldots,d_n,\varphi_n,\theta_n)$$

in a suitable neighborhood of the actually measured values $d_i^{(0)},\varphi_i^{(0)},\theta_i^{(0)},\ i=1,\ldots,n$. By definition,

$$\begin{aligned}
X^{(0)} &= X(d_1^{(0)},\varphi_1^{(0)},\theta_1^{(0)},\ldots,d_n^{(0)},\varphi_n^{(0)},\theta_n^{(0)})\\
Y^{(0)} &= Y(d_1^{(0)},\varphi_1^{(0)},\theta_1^{(0)},\ldots,d_n^{(0)},\varphi_n^{(0)},\theta_n^{(0)})\\
Z^{(0)} &= Z(d_1^{(0)},\varphi_1^{(0)},\theta_1^{(0)},\ldots,d_n^{(0)},\varphi_n^{(0)},\theta_n^{(0)})
\end{aligned}$$

are the desired results of the fitting process.

In what follows, we will assume that the error function E satisfies all necessary differentiability conditions. We are particularly interested in the derivatives

$$\frac{\partial X}{\partial d_i},\ \frac{\partial Y}{\partial d_i},\ \frac{\partial Z}{\partial d_i},\ \ \frac{\partial X}{\partial \varphi_i},\ \frac{\partial Y}{\partial \varphi_i},\ \frac{\partial Z}{\partial \varphi_i},\ \ \frac{\partial X}{\partial \theta_i},\ \frac{\partial Y}{\partial \theta_i},\ \frac{\partial Z}{\partial \theta_i},\ i=1,\ldots,n,$$

because their values, for $d_i=d_i^{(0)},\varphi_i=\varphi_i^{(0)},\theta_i=\theta_i^{(0)},\ i=1,\ldots,n,$

(2.2.2)

$$\begin{aligned}
&\frac{\partial X}{\partial d_i}\Big|^{(0)} = \frac{\partial X}{\partial d_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial X}{\partial \varphi_i}\Big|^{(0)} = \frac{\partial X}{\partial \varphi_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial X}{\partial \theta_i}\Big|^{(0)} = \frac{\partial X}{\partial \theta_i}(d_1^{(0)},\ldots,\theta_n^{(0)})\\
&\frac{\partial Y}{\partial d_i}\Big|^{(0)} = \frac{\partial Y}{\partial d_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial Y}{\partial \varphi_i}\Big|^{(0)} = \frac{\partial Y}{\partial \varphi_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial Y}{\partial \theta_i}\Big|^{(0)} = \frac{\partial Y}{\partial \theta_i}(d_1^{(0)},\ldots,\theta_n^{(0)})\\
&\frac{\partial Z}{\partial d_i}\Big|^{(0)} = \frac{\partial Z}{\partial d_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial Z}{\partial \varphi_i}\Big|^{(0)} = \frac{\partial Z}{\partial \varphi_i}(d_1^{(0)},\ldots,\theta_n^{(0)}),\ \frac{\partial Z}{\partial \theta_i}\Big|^{(0)} = \frac{\partial Z}{\partial \theta_i}(d_1^{(0)},\ldots,\theta_n^{(0)})
\end{aligned}$$

represent the respective sensitivities of the parameters $X^{(0)}, Y^{(0)}, Z^{(0)}$ to perturbations of the indicated data variables.

Implicit differentiation will be used to derive expressions for the sensitivities (2.2.2) from the expression for the error function E. Indeed, the gradient of E with respect to these parameters,

(2.2.3)
$$\nabla_{XYZ}E = \begin{bmatrix} \dfrac{\partial}{\partial X}E(X,Y,Z,d_1,\varphi_1,\theta_1,\ldots,d_n,\varphi_n,\theta_n)\\ \dfrac{\partial}{\partial Y}E(X,Y,Z,d_1,\varphi_1,\theta_1,\ldots,d_n,\varphi_n,\theta_n)\\ \dfrac{\partial}{\partial Z}E(X,Y,Z,d_1,\varphi_1,\theta_1,\ldots,d_n,\varphi_n,\theta_n)\end{bmatrix}$$

vanishes if the parameters X, Y, Z have been minimized with respect to the coordinates d_i, φ_i, θ_i, $i = 1, ..., n$. As we thus substitute for the parameters X, Y, Z their corresponding functions (2.2.1) in the above gradient components, we arrive at a set of derivative functions which are identically zero as functions of the data variables d_i, φ_i, θ_i, $i = 1, ..., n$. In other words, the following derivative expressions,

$$
\begin{aligned}
&\frac{\partial E}{\partial X}(X(d_1,...,\theta_n), Y(d_1,...,\theta_n), Z(d_1,...,\theta_n), d_1,...,\theta_n) \equiv 0 \\
(2.2.4) \qquad &\frac{\partial E}{\partial Y}(X(d_1,...,\theta_n), Y(d_1,...,\theta_n), Z(d_1,...,\theta_n), d_1,...,\theta_n) \equiv 0 \\
&\frac{\partial E}{\partial Z}(X(d_1,...,\theta_n), Y(d_1,...,\theta_n), Z(d_1,...,\theta_n), d_1,...,\theta_n) \equiv 0
\end{aligned}
$$

vanish identically. Then so do the derivatives of these functions, which by the Chain Rule become:

$$
\begin{aligned}
&\frac{\partial^2 E}{\partial X^2}\frac{\partial X}{\partial d_i} + \frac{\partial^2 E}{\partial X \partial Y}\frac{\partial Y}{\partial d_i} + \frac{\partial^2 E}{\partial X \partial Z}\frac{\partial Z}{\partial d_i} + \frac{\partial^2 E}{\partial d_i \partial X} \equiv 0 \\
&\frac{\partial^2 E}{\partial Y \partial X}\frac{\partial X}{\partial d_i} + \frac{\partial^2 E}{\partial Y^2}\frac{\partial Y}{\partial d_i} + \frac{\partial^2 E}{\partial Y \partial Z}\frac{\partial Z}{\partial d_i} + \frac{\partial^2 E}{\partial d_i \partial Y} \equiv 0 \\
&\frac{\partial^2 E}{\partial Z \partial X}\frac{\partial X}{\partial d_i} + \frac{\partial^2 E}{\partial Z \partial Y}\frac{\partial Y}{\partial d_i} + \frac{\partial^2 E}{\partial Z^2}\frac{\partial Z}{\partial d_i} + \frac{\partial^2 E}{\partial d_i \partial Z} \equiv 0.
\end{aligned}
$$

For brevity, we displayed these relationships only for sensitivities with respect to the range variables d_i. Evaluating these functions for the resulting parameters X^0, Y^0, Z^0 and the actual data $d_i^0, \varphi_i^0, \theta_i^0$, yields a numerical $m \times m$ linear system of equations for the sensitivities (2.2.2) with respect to the coordinates d_i. With the notations

$$
\frac{\partial^2 E}{\partial X^2}\Big|^{(0)} = \frac{\partial^2 E}{\partial X^2}(X^{(0)}, Y^{(0)}, Z^{(0)}, d_1^{(0)},...,\theta_n^{(0)}),\ \frac{\partial^2 E}{\partial X \partial Y}\Big|^{(0)} = \frac{\partial^2 E}{\partial X \partial Y}(X^{(0)}, Y^{(0)}, Z^{(0)}, d_1^{(0)},...,\theta_n^{(0)}), \text{ etc.}
$$

this linear system takes the form

$$
\begin{aligned}
&\frac{\partial^2 E}{\partial X^2}\Big|^{(0)}\frac{\partial X}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial X \partial Y}\Big|^{(0)}\frac{\partial Y}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial X \partial Z}\Big|^{(0)}\frac{\partial Z}{\partial d_i}\Big|^{(0)} = -\frac{\partial^2 E}{\partial d_i \partial X}\Big|^{(0)} \\
(2.2.5) \qquad &\frac{\partial^2 E}{\partial Y \partial X}\Big|^{(0)}\frac{\partial X}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial Y^2}\Big|^{(0)}\frac{\partial Y}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial Y \partial Z}\Big|^{(0)}\frac{\partial Z}{\partial d_i}\Big|^{(0)} = -\frac{\partial^2 E}{\partial d_i \partial Y}\Big|^{(0)} \\
&\frac{\partial^2 E}{\partial Z \partial X}\Big|^{(0)}\frac{\partial X}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial Z \partial Y}\Big|^{(0)}\frac{\partial Y}{\partial d_i}\Big|^{(0)} + \frac{\partial^2 E}{\partial Z^2}\Big|^{(0)}\frac{\partial Z}{\partial d_i}\Big|^{(0)} = -\frac{\partial^2 E}{\partial d_i \partial Z}\Big|^{(0)}.
\end{aligned}
$$

The matrix of this linear system may be stated in terms of the Hessian

$$(2.2.6) \qquad \boldsymbol{H}_{XYZ}E = \begin{bmatrix} \frac{\partial^2 E}{\partial X^2} & \frac{\partial^2 E}{\partial X \partial Y} & \frac{\partial^2 E}{\partial X \partial Z} \\ \frac{\partial^2 E}{\partial Y \partial X} & \frac{\partial^2 E}{\partial Y^2} & \frac{\partial^2 E}{\partial Y \partial Z} \\ \frac{\partial^2 E}{\partial Z \partial X} & \frac{\partial^2 E}{\partial Z \partial Y} & \frac{\partial^2 E}{\partial Z^2} \end{bmatrix}$$

of the error function E. The linear system (2.2.5) may thus be written as

$$(2.2.7) \qquad \boldsymbol{H}_{XYZ}E\Big|^{(0)} \begin{bmatrix} \frac{\partial X}{\partial d_i}\Big|^{(0)} \\ \frac{\partial Y}{\partial d_i}\Big|^{(0)} \\ \frac{\partial Z}{\partial d_i}\Big|^{(0)} \end{bmatrix} = -\frac{\partial}{\partial d_i}\nabla_{XYZ}E\Big|^{(0)} \quad ,$$

where again the symbol $\Big|^{(0)}$ is meant to indicate the, -- a posteriory --, substitution by $X^{(0)}, Y^{(0)}, Z^{(0)}$ and the actual data values. The resulting Hessian matrix is positive definite, and therefore nonsingular, at any locally unique minimum of the error function E. The linear system is then solvable and yields the values of the sensitivities (2.2.2) with respect to the variables d_i .

The remaining sensitivities with respect to the variables φ_i and θ_i may be determined from analogous linear systems, based on the same Hessian matrix.

Note that implicit differentiation can be used to determine higher order sensitivities such as

$$\frac{\partial^2 X}{\partial d_i^{\,2}}, \frac{\partial^2 X}{\partial d_l \partial \varphi_j}, \frac{\partial^2 X}{\partial d_i \partial \theta_j}, \frac{\partial^2 X}{\partial \varphi_i^{\,2}},, \frac{\partial^2 X}{\partial \varphi_l \partial \theta_j}, \frac{\partial^2 X}{\partial \theta_l^{\,2}}, \ldots \; .$$

The corresponding linear systems are based on the same Hessian matrix as in (2.2.7) but use different right hand sides.

2.3 Noise Propagation

In, general, data variables d_i, φ_i, θ_i and the parameters X, Y, Z will be considered random variables with expected values $d_i^{(0)}, \varphi_i^{(0)}, \theta_1^{(0)}$ and $X^{(0)}, Y^{(0)}, Z^{(0)}$, respectively. In frequent applications, however, some data variables of the error function will be given “control variables” or “design variables”, and are thus not random. When fitting scanned objects, in particular, it is frequently assumed that the noise in range measurements d_i dominates noise in bearings, which furthermore is difficult to assess. Consequently, only the range coordinates d_i are considered random, while the bearing angles φ_i and θ_i are specified control variables. For scanning instruments, it is generally safe to assume that range variables d_i are independent of each other. The following exposition will be based on these assumptions, again for brevity.

The sensitivities described in the previous section will be instrumental in assessing the effects of data noise on fitted parameters. The well known "Error Propagation Formula" provides first order estimates of the variances (see GUM [24], Chapter 5)

$$
\begin{aligned}
\operatorname{var}(X) &\cong \sum_{i=1}^{n}\left[\frac{\partial X}{\partial d_i}\Big|^{(0)}\right]^2 \operatorname{var}(d_i) \\
\operatorname{var}(Y) &\cong \sum_{i=1}^{n}\left[\frac{\partial Y}{\partial d_i}\Big|^{(0)}\right]^2 \operatorname{var}(d_i) \qquad (2.3.1) \\
\operatorname{var}(Z) &\cong \sum_{i=1}^{n}\left[\frac{\partial Z}{\partial d_i}\Big|^{(0)}\right]^2 \operatorname{var}(d_i) \, .
\end{aligned}
$$

Similarly, one has for the covariances [25],

$$
\begin{aligned}
\operatorname{cov}(X,Y) &\cong \sum_{i=1}^{n}\left[\frac{\partial X}{\partial d_i}\Big|^{(0)} \frac{\partial Y}{\partial d_i}\Big|^{(0)}\right] \operatorname{var}(d_i) = \operatorname{cov}(Y,X) \\
\operatorname{cov}(Y,Z) &\cong \sum_{i=1}^{n}\left[\frac{\partial Y}{\partial d_i}\Big|^{(0)} \frac{\partial Z}{\partial d_i}\Big|^{(0)}\right] \operatorname{var}(d_i) = \operatorname{cov}(Z,Y) \qquad (2.3.2) \\
\operatorname{cov}(Z,X) &\cong \sum_{i=1}^{n}\left[\frac{\partial Z}{\partial d_i}\Big|^{(0)} \frac{\partial X}{\partial d_i}\Big|^{(0)}\right] \operatorname{var}(d_i) = \operatorname{cov}(X,Z) \, .
\end{aligned}
$$

Again, it is here assumed that the coordinate measurements $d_i^{(0)}$ are independent, that is, not correlated, so that their mutual covariances are zero. Note however that, even if the measured quantities $d_i^{(0)}$ are independent, the fitted parameters $X^{(0)}$, $Y^{(0)}$, $Z^{(0)}$ will still be correlated.

In most applications, the condition of homoscedacity is supposed to hold, that is, the variances have the same value within a class of measurements, such as the class d of range measurements,

$$\operatorname{var}(d) = \operatorname{var}(d_i),\ i = 1, \dots n \, .$$

For the special cases of LS and NLS regression, in which the individual errors in our scenario would take the form

$$e_i = d_i - f_i(X, Y, Z, \varphi_i, \theta_i) \, ,$$

a covariance matrix can be approximated in an elegantly simple fashion under homoscedacity as set forth in the general literature, e.g. [5-7, 26, 27]. Unfortunately, the error functions considered here, in particular, the orthogonal error function (Chapter 4) and a portion of the directional error function (Chapter 3) do not fall into this regression category as the required separation of the random variables from the control portion cannot be achieved. It is for this reason, that the more general approach described in Sections 2.2 and 2.3 had to be adopted. A more detailed explanation will be provided in a separate report [23].

3 Directional Fitting of Spheres

3.1 Directional Errors

Introducing the trigonometric quantities $\xi_i, \eta_i, \varsigma_i$, the Cartesian coordinates x_i, y_i, z_i of data points will be expressed in the form

(3.1.1) $$x_i = d_i \cos\varphi_i \cos\theta_i = d_i\xi_i, \quad y_i = d_i \sin\varphi_i \cos\theta_i = d_i\eta_i, \quad z_i = d_i \sin\theta_i = d_i\varsigma_i,$$

where $\xi_i^2 + \eta_i^2 + \varsigma_i^2 = 1$. The vector $(\xi_i, \eta_i, \varsigma_i)$ represents the direction of the scan ray along which the data point $\boldsymbol{P}_i$ was acquired. Next we introduce the quantities:

(3.1.2) $$\begin{aligned} p_i &= X_i\xi_i + Y_i\eta_i + Z_i\varsigma_i \ , \\ q_i^2 &= X^2 + Y^2 + Z^2 - p_i^2 \ , \\ s_i^2 &= R^2 - q_i^2 . \end{aligned}$$

Figures 1 and 2 illustrate the geometric meaning of these quantities.

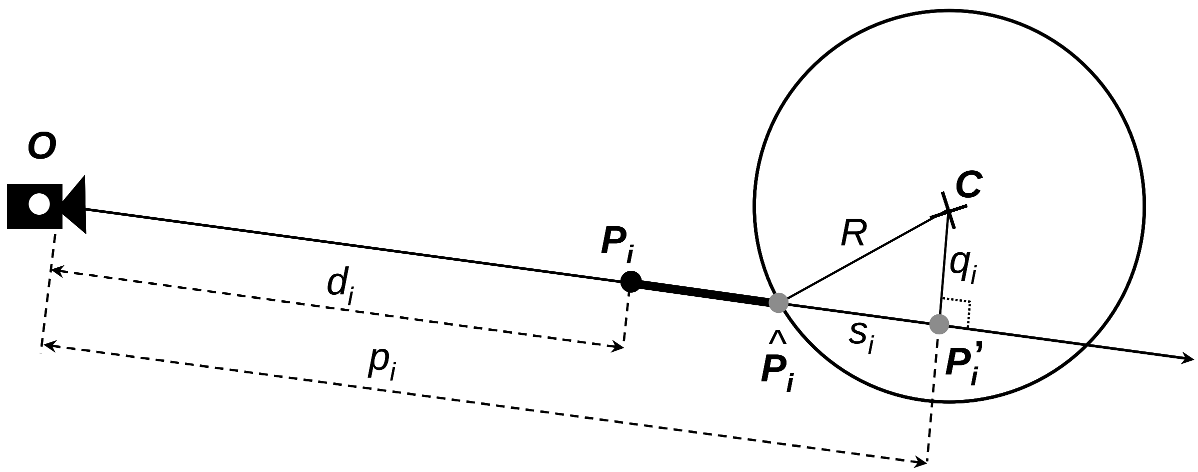

Figure 1. Geometrical interpretation of the directional error function when a scan ray intersects the sphere surface. $\boldsymbol{P_i}$ (marked by dark dot) is the experimental point, light dots mark the theoretical point on the sphere surface $\hat{\boldsymbol{P}}_i$ and the mid-chord point $\boldsymbol{P}_i'$. The length of the bold line segment measures the error f_i defined by (3.1.3).

If the scan ray of data point $\boldsymbol{P}_i$ intersects the virtual sphere centered at $\boldsymbol{C} = [X\ Y\ Z]$, we associate with $\boldsymbol{P}_i$ the midpoint $\boldsymbol{P}_i'$ of the resulting chord. The quantity $p_i = \|\boldsymbol{P}_i'\|$ then represents the distance of that "mid-chord" point from the instrument at the origin $\boldsymbol{O} = [0\ 0\ 0]$. Similarly, $q_i = \|\boldsymbol{P}' - \boldsymbol{C}\| \geq 0$ represents the distance of the mid-chord from the sphere center. Thus

$$q_i < R$$

is the condition for true, that is, non-tangential intersection. The quantities p_i and q_i are side lengths of the right triangle $\Delta \boldsymbol{O}\boldsymbol{P}_i'\boldsymbol{C}$, with its right angle at $\boldsymbol{P}_i'$. Pythagoras thus yields the relation (3.1.2) between p_i^2 and q_i^2. The triangle $\Delta \hat{\boldsymbol{P}}_i \boldsymbol{P}_i'\boldsymbol{C}$, where the theoretical point $\hat{\boldsymbol{P}}_i$ marks the entry point into the sphere, also has a right angle at $\boldsymbol{P}_i'$. The quantity s_i thus represents the length of the half-chord that needs to be subtracted from the distance $p_i = \|\boldsymbol{P}'\|$ to arrive at the desired distance $\|\hat{\boldsymbol{P}}\|$ of the theoretical point from the origin. As a result, the directional error of the data point $\boldsymbol{P}_i$ is given by

(3.1.3) $$f_i = p_i - s_i - d_i \qquad (= \text{“interior error” of } \boldsymbol{P}_i \text{ if } q_i < R)\,.$$

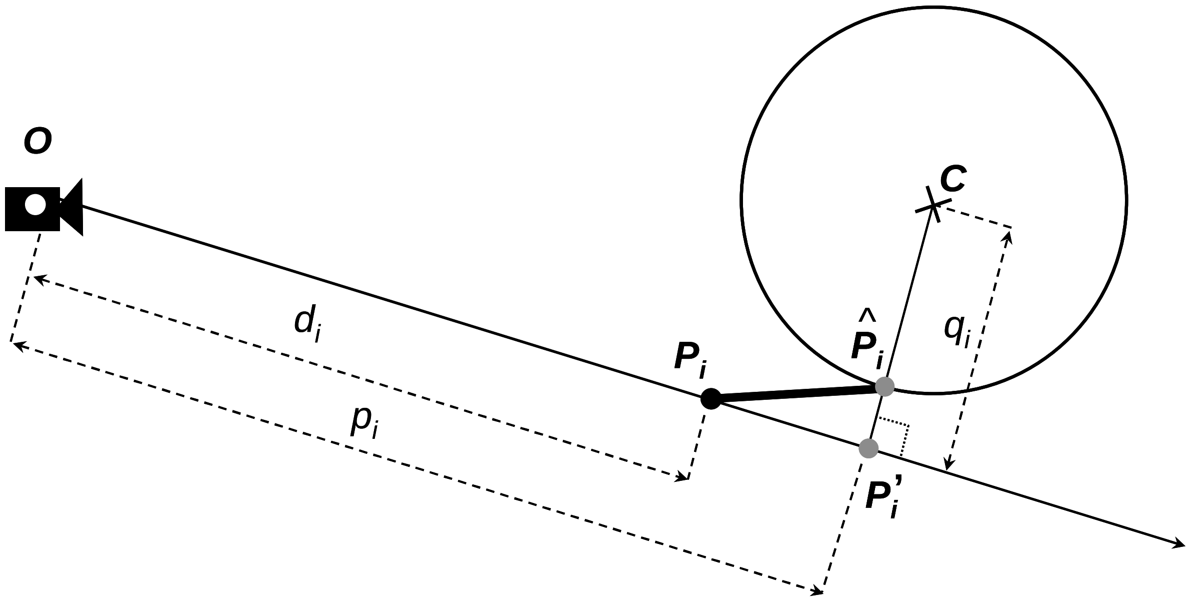

Figure 2. Geometrical interpretation of the directional error function when a scan ray does not intersect the sphere surface. $\boldsymbol{P_i}$ (marked by dark dot) is the experimental point, light dots mark the theoretical point on the sphere surface $\hat{\boldsymbol{P}}_i$ and the point $\boldsymbol{P}_i'$ on a scan ray which is the closest one to the sphere center $\boldsymbol{C}$. The length of the bold line segment measures the error g_i defined by (3.1.4).

On the other hand, if

$$q_i \geq R \ ,$$

then the scan ray of the data point $\boldsymbol{P}_i$ fails to truly intersect the virtual sphere. In that case, and following the general extension principle set forth in Section 2.1, we determine the theoretical point as that point on the virtual sphere which is closest to the scan ray. The line segment which represents the shortest distance between the sphere and the scan ray has to be orthogonal to both the sphere and the scan ray. The line segment thus has to be part of a line through the center of the sphere, and also meet the scan ray at a point $\boldsymbol{P}_i'$ at a right angle. This defines again the right triangle $\Delta \boldsymbol{O}\boldsymbol{P}_i'\boldsymbol{C}$, which we encountered before, and whose side lengths are again p_i and q_i (Fig.2). The desired theoretical point $\hat{\boldsymbol{P}}_i$ thus lies on the side [$\boldsymbol{P}_i'\boldsymbol{O}$] at distance R from center and at distance $q_i - R$ from $\boldsymbol{P}_i'$. The triangle $\Delta \hat{\boldsymbol{P}}_i \boldsymbol{P}_i'\boldsymbol{C}$ is also a right triangle, has side lengths $\left\| \boldsymbol{P}_i' - \boldsymbol{P}_i \right\| = p_i - d_i$ and $\left\| \boldsymbol{P}_i' - \hat{\boldsymbol{P}}_i \right\| = q_i - R$. The length of its hypotenuse $\left\| \hat{\boldsymbol{P}}_i - \boldsymbol{P}_i \right\|$ thus represents the error of the data point $\boldsymbol{P}_i$:

(3.1.4) $$g_i = \sqrt{(p_i - d_i)^2 + (q_i - R)^2} \quad \text{(= "exterior error" of } P_i \text{ if } q_i \geq R\text{)}.$$

(Note that, by Thales' theorem, the locus of all possible points $\boldsymbol{P}_i'$ is the sphere through both the virtual sphere center $\boldsymbol{C}$ and the origin $\boldsymbol{O}$, centered halfway between these two points.)

If $q_i - R = 0$ then $f_i = g_i$, so that the combined error function will be continuous. While the error expression g_i is everywhere twice continuously differentiable, the error expression f_i fails to be so if and only if $s_i = 0$, -- the case of tangential intersection -- , where its gradient with respect to the parameters X, Y, Z is infinite. In these cases, the resulting full error function will also not be differentiable. However, those points will only amount to a closed set of measure zero in parameter space. As a consequence, a gradient based numerical minimization method, such as the often relied on "BFGS" method [28], may still be used [21]. Similarly, the probability of the error function E not being differentiable for the fitted parameters $X^{(0)}, Y^{(0)}, Z^{(0)}$ will be theoretically zero.

We find it convenient, to categorize only a true intersections as a "hit". A tangential intersection is thus considered a "miss", along with all cases in which the virtual sphere is not met at all. Accordingly, we divide the indices i into two sets:

$$U = \{i : q_i < R\} \text{ and } V = \{j : q_j \geq R\}.$$

The combined error function then takes the form

$$E_{direc} = E_{direc}(X, Y, Z, d_1, \varphi_1, ..., d_n, \varphi_n, \theta_n) = \sum_{i \in U} f_i^2 + \sum_{j \in V} g_j^2 \tag{3.1.5}$$

3.2 Derivatives for the Directional Error Function

In this section, we list formulas for the gradients and the Hessians of the individual error functions f_i and g_i with respect to the parameters X, Y, Z, along with the second derivatives with respect to both these parameters and the data variables d_i, φ_i, θ_i. Gradients support optimization methods and are the first step towards determining the above second derivatives, which are needed for the computation of the sensitivities and variances described in Sections 2.3-4. Derivation of these formulas is provided in the Appendix as referenced.

In terms of the individual errors f_i and g_i, the gradients and Hessians of the directional error function are:

$$\nabla_{XYZ} E_{drec} = \sum_{i \in U} \nabla_{XYZ} f_i^2 + \sum_{i \in V} \nabla_{XYZ} g_i^2$$

$$\boldsymbol{H}_{XYZ} E_{drec} = \sum_{i \in U} \boldsymbol{H}_{XYZ} f_i^2 + \sum_{i \in V} \boldsymbol{H}_{XYZ} g_i^2 .$$

The gradients are linear combinations of the vectors

(3.2.1) $$\boldsymbol{U} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Lambda}_i = \begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix},$$

namely (see (A.2.6) and (A.2.7) in Appendix)

(3.2.2) $$\frac{1}{2}\nabla_{XYZ} f_i^2 = \frac{f_i}{s_i}\boldsymbol{U} - \frac{f_i(f_i + d_i)}{s_i}\boldsymbol{\Lambda}_i \ , \quad \frac{1}{2}\nabla_{XYZ} g_i^{\ 2} = (1 - \frac{R}{q_i})\boldsymbol{U} + (\frac{Rp_i}{q_i} - d_i)\boldsymbol{\Lambda}_i$$

Similarly, the Hessian matrices are linear combinations of the following four symmetric matrices:

(3.2.3) $$\boldsymbol{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ (Identity)},$$

$$\boldsymbol{U}\boldsymbol{U}^T = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \begin{bmatrix} X & Y & Z \end{bmatrix} = \begin{bmatrix} X^2 & XY & XZ \\ YX & Y^2 & YZ \\ ZX & ZY & Z^2 \end{bmatrix},$$

$$\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \begin{bmatrix} \xi_i & \eta & \varsigma_i \end{bmatrix} + \begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix} \begin{bmatrix} X & Y & Z \end{bmatrix} = \begin{bmatrix} X\xi_i + \xi_i X & X\eta_i + \xi_i Y & X\varsigma_i + \xi_i Z \\ Y\xi_i + \eta_i X & Y\eta_i + \eta_i Y & Y\varsigma_i + \eta_i Z \\ Z\xi_i + \varsigma_i X & Z\eta_i + \varsigma_i Y & Z\varsigma_i + \varsigma_i Z \end{bmatrix},$$

$$\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T = \begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix} \begin{bmatrix} \xi_i & \eta & \varsigma_i \end{bmatrix} = \begin{bmatrix} \xi_i^2 & \eta_i\xi_i & \xi_i\varsigma_i \\ \eta_i\xi_i & \eta_i^2 & \eta_i\varsigma_i \\ \varsigma_i\xi_i & \varsigma_i\eta_i & \varsigma_i^2 \end{bmatrix}.$$

Thus, (see (A.2.11) and (A.2.12))

(3.2.4) $$\frac{1}{2}\boldsymbol{H}_{XYZ} f_i^2 = \left(\frac{p_i - d_i}{s_i} - 1\right)\boldsymbol{I} + \left(\frac{p_i - d_i}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T - \left(\frac{p_i(p_i - d_i)}{s_i^3} - \frac{1}{s_i}\right)(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + \left(\frac{(p_i^2 - s_i^2)(p_i - d_i)}{s_i^3} + \frac{2(p_i - s_i)}{s_i}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T$$

$$\frac{1}{2}\boldsymbol{H}_{XYZ} g_i^2 = \left(1 - \frac{R}{q_i}\right)\boldsymbol{I} + \frac{R}{q_i^3}\boldsymbol{U}\boldsymbol{U}^T - \frac{Rp_i}{q_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + R\left(\frac{X^2 + Y^2 + Z^2}{q_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T .$$

Evaluated for optimal parameters $X^{(0)}, Y^{(0)}, Z^{(0)}$ and actual data points $\boldsymbol{P}_i = [d_i^{(0)}\ \varphi_i^{(0)}\ \theta_i^{(0)}]$, these Hessian matrices support the left hand side of linear systems (2.2.7) for the corresponding sensitivities. For the right-hand sides of those systems, we have for the range variables d_i ,

$$\nabla_{XYZ}\frac{\partial}{\partial d_i}E_{drec} = \sum_{i\in U}\nabla_{XYZ}\frac{\partial f_i^2}{\partial d_i} + \sum_{i\in V}\nabla_{XYZ}\frac{\partial g_i^2}{\partial d_i}$$

where (see (A.3.1) and (A.3.2))

(3.2.5) $$\frac{1}{2}\nabla_{XYZ}\frac{\partial f_i^2}{\partial d_i} = -\frac{1}{s_i}\boldsymbol{U} - \frac{p_i - s_i}{s_i}\boldsymbol{\Lambda}_i , \qquad \frac{1}{2}\nabla_{XYZ}\frac{\partial g_i^2}{\partial d_i} = -\boldsymbol{\Lambda}_i .$$

For the bearing variables φ , θ, the individual derivatives in

$$\nabla_{XYZ}\frac{\partial}{\partial \varphi_i}E_{drec} = \sum_{i\in U}\nabla_{XYZ}\frac{\partial f_i^2}{\partial \varphi_i} + \sum_{i\in V}\nabla_{XYZ}\frac{\partial g_i^2}{\partial \varphi_i} ,$$

$$\nabla_{XYZ}\frac{\partial}{\partial \theta_i}E_{drec} = \sum_{i\in U}\nabla_{XYZ}\frac{\partial f_i^2}{\partial \theta_i} + \sum_{i\in V}\nabla_{XYZ}\frac{\partial g_i^2}{\partial \theta_i} .$$

are multiples of the vectors

(3.2.6) $$\frac{\partial}{\partial \varphi_i}\boldsymbol{\Lambda}_i = \begin{bmatrix} -\eta_i \\ \xi_i \\ 0 \end{bmatrix} , \qquad \frac{\partial}{\partial \theta_i}\boldsymbol{\Lambda}_i = \begin{bmatrix} \alpha_i \\ \beta_i \\ \gamma_i \end{bmatrix} ,$$

where $\alpha_i = -\cos\varphi_i \sin\theta_i$, $\beta_i = -\sin\varphi_i \sin\theta_i$, $\gamma_i = \cos\theta_i$. Thus

(3.2.7) $$\frac{1}{2}\nabla_{XYZ}\frac{\partial f_i^2}{\partial \varphi_i} = \boldsymbol{\Gamma}_i(f_i^2)\begin{bmatrix}-\eta_i\\ \xi_i\\ 0\end{bmatrix}, \quad \frac{1}{2}\nabla_{XYZ}\frac{\partial g_i^2}{\partial \varphi_i} = \boldsymbol{\Gamma}_i(g_i^2)\begin{bmatrix}-\eta_i\\ \xi_i\\ 0\end{bmatrix}$$

(3.2.8) $$\frac{1}{2}\nabla_{XYZ}\frac{\partial f_i^2}{\partial \theta_i} = \boldsymbol{\Gamma}_i(f_i^2)\begin{bmatrix}\alpha_i\\ \beta_i\\ \gamma_i\end{bmatrix}, \quad \frac{1}{2}\nabla_{XYZ}\frac{\partial g_i^2}{\partial \theta_i} = \boldsymbol{\Gamma}_i(g_i^2)\begin{bmatrix}\alpha_i\\ \beta_i\\ \gamma_i\end{bmatrix},$$

where the two pre-multiplying matrices are given by

(3.2.9)
$$\boldsymbol{\Gamma}_i(f_i^2) = \left(\frac{1}{s_i} - \frac{p_i(p_i-d_i)}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T + (p_i - s_i)\left(\frac{(p_i+s_i)(p_i-d_i)}{s_i^2} - \frac{2}{s_i}\right)\boldsymbol{\Lambda}_i\boldsymbol{U}^T + (p_i - s_i)\left(1 - \frac{p_i - d_i}{s_i}\right)\boldsymbol{I},$$

$$\boldsymbol{\Gamma}_i(g_i^2) = \left(-\frac{Rp_i}{q_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T + R\left(\frac{X^2+Y^2+Z^2}{q_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{U}^T + \left(\frac{Rp_i}{q_i} - d_u\right)\boldsymbol{I}\ .$$

As

(3.2.10) $$\boldsymbol{\Lambda}_i^T\begin{bmatrix}-\eta_i\\ \xi_i\\ 0\end{bmatrix} = \boldsymbol{0} \ \text{and}\ \ \boldsymbol{\Lambda}_i^T\begin{bmatrix}\alpha_i\\ \beta_i\\ \gamma_i\end{bmatrix} = \boldsymbol{0}\ ,$$

the above matrices may be replaced in (3.2.7) and (3.2.8), respectively, by the following symmetrized versions:

(3.2.11)
$$\boldsymbol{\Gamma}_i^S(f_i^2) = \left(\frac{1}{s_i} - \frac{p_i(p_i-d_i)}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T + (p_i - s_i)\left(\frac{(p_i+s_i)(p_i-d_i)}{s_i^2} - \frac{2}{s_i}\right)(\boldsymbol{\Lambda}_i\boldsymbol{U}^T + \boldsymbol{U}\boldsymbol{\Lambda}_i^T) +$$
$$(p_i - s_i)\left(1 - \frac{p_i - d_i}{s_i}\right)\boldsymbol{I},$$

$$\boldsymbol{\Gamma}_i^S(g_i^2) = \left(-\frac{Rp_i}{q_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T + R\left(\frac{X^2+Y^2+Z^2}{q_i^3}\right)(\boldsymbol{\Lambda}_i\boldsymbol{U}^T + \boldsymbol{U}\boldsymbol{\Lambda}_i^T) + \left(\frac{Rp_i}{q_i} - d_u\right)\boldsymbol{I} .$$

4 Orthogonal Fitting of Spheres

Here, the theoretical point $\hat{\boldsymbol{P}}_i$, that is, the point on the sphere which is closest to the data point $\boldsymbol{P}_i = [x_i \quad y_i \quad z_i]$, defines the individual error

$$h_i = \left\|\hat{\boldsymbol{P}}_i - \boldsymbol{P}_i\right\| = \left\|\boldsymbol{C} - \boldsymbol{P}_i\right\| - R = w_i - R$$

with respect to the sphere center $\boldsymbol{C}$ and the radius R. We thus represent the orthogonal fitting approach by the full error function

(4.1.1) $$E_{orth} = \sum_{i=1}^{n} h_I^2 = \sum_{i=1}^{n}(w_i - R)^2 = w_i^2 - 2Rw_i + R^2 .$$

Consistent with the generation of point clouds by scanning from a single instrument location, and as discussed before, the underlying coordinate frames are again considered polar with the instrument location at the origin. For an analytic discussion of the orthogonal error function in terms of Cartesian data see [11].

With the notation (3.1.1) and the definition (3.1.2) of the auxiliary quantitity p_i ,

$$x_i = d_i\cos\varphi_i\cos\theta_i = d_i\xi_i, \quad y_i = d_i\sin\varphi_i\cos\theta_i = d_i\eta_i, \quad z_i = d_i\sin\theta_i = d_i\xi_i,$$

we have

(4.1.2) $$w_i^2 = (X - x_i)^2 + (Y - y_i)^2 + (Z - z_i)^2 = (X^2 + Y^2 + Z^2) - 2d_i p_i + d_i^2 .$$

A key vector, in which gradients and Hessians of the individual orthogonal error squares h_i^2 may be expressed, is given by

(4.1.3) $$\boldsymbol{W}_i = \begin{bmatrix} X - x_i \\ Y - y_i \\ Z - z_i \end{bmatrix} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} - d_i\begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix} = \boldsymbol{U} - d_i\boldsymbol{\Lambda}_i ,$$

as $\boldsymbol{W}_i^T \boldsymbol{W}_i = w_i^2$. Also (see (A.4.3) and (A.4.5)),

(4.1.4) $$\frac{1}{2}\nabla_{XYZ} h_i^2 = \left(1 - \frac{R}{w_i}\right)\boldsymbol{W}_i$$

and

(4.1.5) $$\frac{1}{2}\boldsymbol{H}_{XYZ} h_i^2 = \left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{R}{w_i^3} W_i W_i^T \ .$$

For the derivatives which define the right-hand sides of the linear system (2.2.7), we have first:

$$\nabla_{XYZ} \frac{\partial}{\partial d_i} E_{orth} = \sum_{i=1}^{n} \nabla_{XYZ} \frac{\partial h_i^{\,2}}{\partial d_i}$$

with (see (A.5.2))

(4.1.6) $$\frac{1}{2}\nabla_{XYZ} \frac{\partial h_i^2}{\partial d_i} = -\frac{R}{w_i^3}(p_i - d_i)\boldsymbol{W}_i - \left(1 - \frac{R}{w_i}\right)\boldsymbol{\Lambda}_i \ .$$

Again, the corresponding mixed derivatives with respect to the bearing variables φ_i, θ_i are multiples of the vectors $\frac{\partial}{\partial \varphi_i}\boldsymbol{\Lambda}_i$ and $\frac{\partial}{\partial \theta_i}\boldsymbol{\Lambda}_i$, defined in (3.2.6). Their common multiplier is the matrix

(4.1.7) $$\boldsymbol{\Gamma}_i(h_i^2) = -d_i\left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{Rd_i}{w_i^3}\boldsymbol{W}_i\boldsymbol{U}^T ,$$

which, in analogy to (3.2.11), may be replaced also by its symmetrized form,

(4.1.8) $$\frac{1}{2}\boldsymbol{\Gamma}_i^S(h_i^2) = -d_i\left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{Rd_i}{w_i^3}\boldsymbol{W}_i\boldsymbol{W}_i^T \ .$$

Thus

(4.2.5) $$\frac{1}{2}\nabla_{XYZ} \frac{\partial h_i^2}{\partial \varphi_i} = \boldsymbol{\Gamma}_i(h_i^2)\begin{bmatrix} -\eta_i \\ \xi_i \\ 0 \end{bmatrix} = \boldsymbol{\Gamma}_i^S(h_i^2)\begin{bmatrix} -\eta_i \\ \xi_i \\ 0 \end{bmatrix}$$

and

(4.2.6)
$$\frac{1}{2}\nabla_{XYZ}\frac{\partial h_i^2}{\partial \theta_i} = \boldsymbol{\Gamma}_i(h_i^2)\begin{bmatrix}\alpha_i\\ \beta_i\\ \gamma_i\end{bmatrix} = \boldsymbol{\Gamma}_i^s(h_i^2)\begin{bmatrix}\alpha_i\\ \beta_i\\ \gamma_i\end{bmatrix} .$$

This concludes the main part of the report. It is followed by the Appendix in which details about the derivation of the key formulas are provided.

Appendix A: Determination of Derivative Formulas Used for Calculating Sensitivities

Here, we provide step by step developments of the derivative formulas referred to in Chapters 3 and 4 for the purpose of determining the parameter sensitivities for directional and orthogonal fitting. In Section A.2, the gradient $\nabla_{XYZ}E_{direc}$ and Hessian $\boldsymbol{H}_{XYZ}E_{drec}$ of the directional error function are at issue. The Hessian provides the matrix for the corresponding linear system (2.2.7). Also for the directional error function, the derivatives of both parameters and data variables,

$$\frac{\partial}{\partial d_i}\nabla_{XYZ}E = \nabla_{XYZ}\frac{\partial E}{\partial d_i} \,,\ \frac{\partial}{\partial \varphi_i}\nabla_{XYZ}E = \nabla_{XYZ}\frac{\partial E}{\partial \varphi_i} \,,\ \frac{\partial}{\partial \theta_i}\nabla_{XYZ}E = \nabla_{XYZ}\frac{\partial E}{\partial \theta_i} \ ,$$

are derived in Section A.3, furnishing the right hand sides of these systems. Finally, Section A.4 provides the analogous information in the case of orthogonal fitting.

A.1 General Considerations

In what follows, the calculation of gradients ∇_{XYZ} and Hessians $\boldsymbol{H}_{XYZ}$ will often be based on the following straightforward reformulations of product and chain rules:

(A.1.1)
$$\nabla_{XYZ}b(a) = b'(a)\nabla_{XYZ}a \ ,$$

$$\nabla_{XYZ}ab = a\nabla_{XYZ}b + b\nabla_{XYZ}a \ ,$$

$$\nabla_{XYZ}a^2 = 2a\nabla_{XYZ}a \ ,$$

$$\nabla_{XYZ}a = \nabla_{XYZ}\sqrt{a^2} = \frac{1}{2}\frac{1}{a}\nabla_{XYZ}\sqrt{a^2} \ ,$$

and

(A.1.2)
$$\boldsymbol{H}_{XYZ}b(a) = b''(a)\nabla_{XYZ}a\nabla_{XYZ}^T a + b'(a)\boldsymbol{H}_{XYZ}a \,,$$

$$\boldsymbol{H}_{XYZ}ab = \nabla_{XYZ}a\nabla_{XYZ}^T b + \nabla_{XYZ}b\nabla_{XYZ}^T a + a\boldsymbol{H}_{XYZ}b + b\boldsymbol{H}_{XYZ}a \ ,$$

$$\boldsymbol{H}_{XYZ}a^2 = 2\nabla_{XYZ}a\nabla^T_{XYZ}a + 2a\boldsymbol{H}_{XYZ}a \ ,$$

$$\boldsymbol{H}_{XYZ}a = \boldsymbol{H}_{XYZ}\sqrt{a^2} = -\frac{1}{4}\frac{1}{a^3}\nabla_{XYZ}a^2\nabla^T_{XYZ}a^2 + \frac{1}{2}\frac{1}{a}\boldsymbol{H}_{XYZ}a^2 \ .$$

These formulas are straightforward reformulations of product and chain rules, and will not always be referred in what follows.

A.2 Gradients and Hessians of the Directional Error Functions

Recall the directional error function

$$E_{drec} == \sum_{i\in U} f_i^{\,2} + \sum_{i\in V} g_i^{\,2}$$

with individual errors (3.1.3-4),

$$f_i = p_i - s_i - d_i \ , \ \ g_i = \sqrt{(p_i - d_i)^2 + (q_i - R)^2} \ ,$$

based on the auxiliary quantities p_i, q_i, s_i (3.1.2) and the direction cosines (3.1.1)

$$\xi_i = \cos\varphi_i \cos\theta_i \, , \ \ \eta_i = \sin\varphi_i \cos\theta_i \, , \ \ \varsigma_i = \sin\theta_i \ .$$

Again, all gradients ∇_{XYZ} determined in this Section will be linear combinations of the two vectors,

$$\boldsymbol{U} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \quad \text{and} \quad \boldsymbol{\Lambda}_i = \begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix},$$

which were introduced in Section 3.2. Using (A.1.1) where indicated, we note:

(A.2.1) $$\nabla_{XYZ}p_i = \nabla_{XYZ}(X\xi_i + Y\eta_i + Z\varsigma_i) = \boldsymbol{\Lambda}_i \ , \quad \nabla_{XYZ}p_i^2 = 2p_i\boldsymbol{\Lambda}_i \ ,$$

$$\nabla_{XYZ}q_i^2 = \nabla_{XYZ}(X^2 + Y^2 + Z^2) - \nabla_{XYZ}p_i^2 = 2[\boldsymbol{U} - p_i\boldsymbol{\Lambda}_i] \ ,$$

$$\nabla_{XYZ}q_i = \nabla_{XYZ}\sqrt{q_i^{\,2}} = \frac{1}{2}\frac{1}{q_i}\nabla_{XYZ}q_i^{\,2} = \frac{1}{q_i}[\boldsymbol{U} - p_i\boldsymbol{\Lambda}_i] \ ,$$

$$\nabla_{XYZ} s_i^{\,2} = \nabla_{XYZ}(R^2 - q_i^2) = -\nabla_{XYZ} q_i^{\,2} = -2\left[\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i\right] ,$$

$$\nabla_{XYZ} s_i = \nabla_{XYZ}\sqrt{s_i^{\,2}} = \frac{1}{2}\frac{1}{s_i}\nabla_{XYZ} s_i^{\,2} = -\frac{1}{s_i}\left[\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i\right] ,$$

$$\nabla_{XYZ}\frac{1}{s_i} = -\frac{1}{s_i^{\,2}}\nabla_{XYZ} s_i = \frac{1}{s_i^{\,3}}\left[\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i\right] .$$

All Hessians $\boldsymbol{H}_{XYZ}$ determined in this section will be linear combinations of the four matrices (3.2.4). Again we begin with the auxiliary quantities:

(A.2.2) $\quad \boldsymbol{H}_{XYZ}\, p_i = 0 , \qquad \boldsymbol{H}_{XYZ}\, p_i^2 = 2\nabla_{XYZ}\, p_i \nabla_{XYZ}^T\, p_i = 2\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T$ by (A.1.2),

$$\boldsymbol{H}_{XYZ} q_i^2 = \boldsymbol{H}_{XYZ}(X^2 + Y^2 + Z^2) - \boldsymbol{H}_{XYZ}\, p_i^2 = 2\left(\boldsymbol{I} - \boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T\right) ,$$

$$\boldsymbol{H}_{XYZ} s_i^2 = -\boldsymbol{H}_{XYZ} q_i^2 = -2\left(\boldsymbol{I} - \boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T\right) ,$$

From Hessians of q_i^2, s_i^2 we pass to Hessians of q_i , s_i, using (A.1.2)

$$\begin{aligned}
\boldsymbol{H}_{XYZ} q_i &= \boldsymbol{H}_{XYZ}\sqrt{q_i^2} = \frac{-1}{4}\frac{1}{q_i^3}\nabla_{XYZ} q_i^2 \nabla_{XYZ}^T q_i^2 + \frac{1}{2}\frac{1}{q_i}\boldsymbol{H}_{XYZ} q_i^2 \\
&= -\frac{1}{q_i^3}\left(\boldsymbol{U} - p_i\boldsymbol{\Lambda}_i\right)\left(\boldsymbol{U} - p_i\boldsymbol{\Lambda}_i\right)^T + \frac{1}{q_i}\left(\boldsymbol{I} - \boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T\right) \\
&= -\frac{1}{q_i^3}\boldsymbol{U}\boldsymbol{U}^T + \frac{p_i}{q_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i + \boldsymbol{\Lambda}_i\boldsymbol{U}) - \frac{p_i^2}{q_i^3}\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T + \frac{1}{q_i}(\boldsymbol{I} - \boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T).
\end{aligned}$$

Thus

(A.2.3) $\quad \boldsymbol{H}_{XYZ} q_i = \dfrac{1}{q_i}\boldsymbol{I} - \dfrac{1}{q_i^3}\boldsymbol{U}\boldsymbol{U}^T + \dfrac{p_i}{q_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i + \boldsymbol{\Lambda}_i\boldsymbol{U}) - \left(\dfrac{p_i^2}{q_i^3} + \dfrac{1}{q_i}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T .$

Concerning the last term, note

$$\frac{p_i^2}{q_i^3} + \frac{1}{q_i} = \frac{p_i^2 + q_i^2}{q_i^3} = \frac{X^2 + Y^2 + Z^2}{q_i^3} .$$

Similarly, by (A.1.2),

$$\boldsymbol{H}_{XYZ} s_i = \boldsymbol{H}_{XYZ} \sqrt{s_i^2} = \frac{-1}{4}\frac{1}{s_i^3} \nabla_{XYZ} s_i^2 \nabla_{XYZ}^T s_i^2 + \frac{1}{2}\frac{1}{s_i} \boldsymbol{H}_{XYZ} s_i^2$$

$$= -\frac{1}{s_i^3} (\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i)(\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i)^T - \frac{1}{s_i}(\boldsymbol{I} - \boldsymbol{\Lambda}_i \boldsymbol{\Lambda}_i^T)$$

$$= -\frac{1}{s_i^3} \boldsymbol{U}\boldsymbol{U}^T + \frac{p_i}{s_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i + \boldsymbol{\Lambda}_i \boldsymbol{U}) - \frac{p_i^2}{s_i^3} \boldsymbol{\Lambda}_i \boldsymbol{\Lambda}_i^T - \frac{1}{s_i}(\boldsymbol{I} - \boldsymbol{\Lambda}_i \boldsymbol{\Lambda}_i^T).$$

Thus

(A.2.4) $$\boldsymbol{H}_{XYZ} s_i = -\frac{1}{s_i}\boldsymbol{I} - \frac{1}{s_i^3}\boldsymbol{U}\boldsymbol{U}^T + \frac{p_i}{s_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i + \boldsymbol{\Lambda}_i \boldsymbol{U}) + \left(\frac{1}{s_i} - \frac{p_i^2}{s_i^3}\right)\boldsymbol{\Lambda}_i \boldsymbol{\Lambda}_i^T .$$

Concerning the last term, note

$$\frac{1}{s_i} - \frac{p_i^2}{s_i^3} = \frac{s_i^2 - p_i^2}{q_i^3} = \frac{R^2 - q_i^2 - p_i^2}{q_i^3} = \frac{R^2 - (X^2 + Y^2 + Z^2)}{q_i^3} = -\frac{X^2 + Y^2 + Z^2 - R^2}{q_i^3} .$$

From the above, we derive derivative expressions involving the errors f_i and g_i:

(A.2.5)
$$\nabla_{XYZ} f_i = \nabla_{XYZ} p_i - \nabla_{XYZ} s_i = \boldsymbol{\Lambda}_i + \frac{1}{s_i}(\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i)$$
$$= \frac{1}{s_i}\boldsymbol{U} - \frac{p_i - s_i}{s_i}\boldsymbol{\Lambda}_i = \frac{1}{s_i}\boldsymbol{U} - \frac{f_i + d_i}{s_i}\boldsymbol{\Lambda}_i$$

(A.2.6) $$\frac{1}{2}\nabla_{XYZ} f_i^2 = f_i \nabla_{XYZ} f_i = \frac{f_i}{s_i}\boldsymbol{U} - \frac{f_i(f_i + d_i)}{s_i}\boldsymbol{\Lambda}_i$$

For the external portion of the error function, we find

$$\nabla_{XYZ} g_i^2 = 2(p_i - d_i)\nabla_{XYZ} p_i + 2(q_i - R)\nabla_{XYZ} q_i = 2(p_i - d_i)\boldsymbol{U} + \frac{2(q_i - R)}{q_i}(\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i)$$
$$= \frac{2(q_i - R)}{q_i}\boldsymbol{U} + \frac{2(p_i - d_i)q_i - 2(q_i - R)p_i}{q_i}\boldsymbol{\Lambda}_i$$

or

(A.2.7) $$\frac{1}{2}\nabla_{XYZ} g_i^2 = (1 - \frac{R}{q_i})\boldsymbol{U} + (\frac{Rp_i}{q_i} - d_i)\boldsymbol{\Lambda}_i$$

and by (A.1.1),

(A.2.8) $$\nabla_{XYZ} g_i = \nabla_{XYZ} \sqrt{g_i^{\,2}} = \frac{1}{2}\frac{1}{g_i}\nabla_{XYZ} g_i^{\,2} = \frac{1}{q_i g_i}\big((q_i - R)\boldsymbol{U} + (R p_i - d_i q_i)\boldsymbol{\Lambda}_i\big) .$$

Moving to the second derivatives, we find

(A.2.9) $$\boldsymbol{H}_{XYZ} f_i = -\boldsymbol{H}_{XYZ} s_i = \frac{1}{s_i}\boldsymbol{I} + \frac{1}{s_i^3}UU^T - \frac{p_i}{s_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + \left(\frac{1}{s_i} - \frac{p_i^2}{s_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T .$$

Next, we introduce the matrix

$$\begin{aligned} \boldsymbol{G}_{XYZ} f_i &= \nabla_{XYZ} f_i \nabla_{XYZ}^T f_i = \frac{1}{s_i^2}\big(\boldsymbol{U} - (p_i - s_i)\boldsymbol{\Lambda}_i\big)\big(\boldsymbol{U} - (p_i - s_i)\boldsymbol{\Lambda}_i\big)^T \\ &= \frac{1}{s_i^2}\boldsymbol{U}\boldsymbol{U}^T - \frac{p_i - s_i}{s_i^2}(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + \frac{(p_i - s_i)^2}{s_i^2}\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T \end{aligned} .$$

Also by (A2.9),

$$f_i \boldsymbol{H}_{XYZ} f_i = \frac{f_i}{s_i}\boldsymbol{I} + \frac{f_i}{s_i^3}\boldsymbol{U}\boldsymbol{U}^T - \frac{f_i p_i}{s_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + \frac{f_i(p_i^2 - s_i^2)}{s_i^3}\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T .$$

By (A.1.2) , $\boldsymbol{H}_{XYZ} f_i^{\,2} = 2\boldsymbol{G}_{XYZ} f_i + 2 f_i \boldsymbol{H}_{XYZ} f_i$. Thus

(A.2.10) $$\begin{aligned} \frac{1}{2}\boldsymbol{H}_{XYZ} f_i^{\,2} &= \frac{f_i}{s_i}\boldsymbol{I} + \left(\frac{1}{s_i^2} + \frac{f_i}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T - \left(\frac{p_i - s_i}{s_i^2} + \frac{f_i p_i}{s_i^3}\right)(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) \\ &\quad + \left(\frac{(p_i - s_i)^2}{s_i^2} + \frac{f_i(p_i^2 - s_i^2)}{s_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T . \end{aligned}$$

Expressing $f_i = p_i - s_i - d_i$ yields

$$\frac{1}{s_i^2} + \frac{f_i}{s_i^3} = \frac{s_i + f_i}{s_i^3} = \frac{p_i - d_i}{s_i^3}$$

$$\frac{p_i - s_i}{s_i^2} + \frac{f_i p_i}{s_i^3} = \frac{(p_i - s_i)s_i + f_i p_i}{s_i^3} = \frac{p_i s_i - s_i^2 + p_i^2 - p_i s_i - p_i d_i}{s_i^3} = \frac{p_i(p_i - d_i)}{s_i^3} - \frac{1}{s_i}$$

$$\frac{(p_i - s_i)^2}{s_i^3} + \frac{f_i(p_i^2 - s_i^2)}{s_i^3} = \frac{p_i^2 s_i - 2p_i s_i^2 + s_i^3 + p_i^3 - p_i s_i^2 - s_i p_i^2 + s_i^3 - p_i^2 d_i + d_i s_i^2}{s_i^3}$$
$$= \frac{(p_i^3 - p_i^2 d_i) - (p_i s_i^2 - d_i s_i^2) - 2p_i s_i^2 + 2s_i^3}{s_i^3}$$
$$= \frac{(p_i^2 - s_i^2)(p_i - d_i) - 2(p_i - s_i)s_i^2}{s_i^3}$$

From these relations, we find the alternate expression

(A.2.11)
$$\begin{aligned}\frac{1}{2}\boldsymbol{H}_{XYZ} f_i^2 &= \left(\frac{p_i - d_i}{s_i} - 1\right)\boldsymbol{I} + \left(\frac{p_i - d_i}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T \\ &- \left(\frac{p_i(p_i - d_i)}{s_i^3} - \frac{1}{s_i}\right)(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) \\ &+ \left(\frac{(p_i^2 - s_i^2)(p_i - d_i)}{s_i^3} + \frac{2(p_i - s_i)}{s_i}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T.\end{aligned}$$

which duplicates the first portion of (3.2.1).

We move now to the external portion g_i of the error function. Note that the following Hessians vanish:

$$\boldsymbol{H}_{XYZ}\, p_i d_i,\ \boldsymbol{H}_{XYZ}\, d_i^2,\ \boldsymbol{H}_{XYZ}\, R^2.$$

Thus

$$\begin{aligned}\boldsymbol{H}_{XYZ}\, g_i^2 &= \boldsymbol{H}_{XYZ}\left((p_i - d_i)^2 + (q_i - R)^2\right) = \boldsymbol{H}_{XYZ}(p_i^2 - 2p_i d_i + d_i^2 + q_i^2 - 2q_i R + R^2) \\ &= \boldsymbol{H}_{XYZ}(p_i^2 + q_i^2 - 2Rq_i) = \boldsymbol{H}_{XYZ}(X^2 + Y^2 + Z^2 - 2Rq_i) = 2\boldsymbol{I} - 2R\boldsymbol{H}_{XYZ}\, q_i\end{aligned}$$

and by (A.2.2),

(A.2.12)
$$\boldsymbol{H}_{XYZ}\, g_i^2 = \left(1 - \frac{R}{q_i}\right)\boldsymbol{I} + \frac{R}{q_i^3}\boldsymbol{U}\boldsymbol{U}^T - \frac{Rp_i}{q_i^3}(\boldsymbol{U}\boldsymbol{\Lambda}_i^T + \boldsymbol{\Lambda}_i\boldsymbol{U}^T) + R\left(\frac{X^2 + Y^2 + Z^2}{q_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{\Lambda}_i^T.$$

This establishes the second portion of (3.2.1).

A.3 Mixed Derivatives of the Directional Error Function

The right-and-sides of the system of linear equations (2.2.7) are at issue. They require the negatives mixed derivatives of the form

$$\frac{\partial}{\partial *}\nabla_{XYZ} E_{direc} = \nabla_{XYZ} \frac{\partial}{\partial *} E_{direc} \ ,$$

where $*$ indicates a data variable of the error function. We first consider the data variable d_i. Note, in this context,

$$\nabla_{XYZ} \frac{\partial f_i}{\partial d_i} = \nabla_{XYZ}(-1) = 0 \,, \quad \nabla_{XYZ} \frac{\partial f_i^{\,2}}{\partial d_i} = \nabla_{XYZ}\left(2 f_i \frac{\partial f_i}{\partial d_i}\right) = \nabla_{XYZ}(-2 f_i) = -2\left(\nabla_{XYZ} p_i - \nabla_{XYZ} s_i\right) \ .$$

Thus by (A.2.1),

(A.3.1)
$$\frac{1}{2}\nabla_{XYZ} \frac{\partial f_i^{\,2}}{\partial d_i} = -\boldsymbol{\Lambda}_i - \frac{1}{s_i}(\boldsymbol{U} - p_i \boldsymbol{\Lambda}_i) = -\frac{1}{s_i}(\boldsymbol{U} + (p_i - s_i)\boldsymbol{\Lambda}_i) \ .$$

Similarly,

$$\nabla_{XYZ} \frac{\partial g_i^2}{\partial d_i} = \nabla_{XYZ} \frac{\partial}{\partial d_i}\left((p_i - d_i)^2 + (q_i - R)^2\right) = -2\left(\nabla_{XYZ}(p_i - d_i)\right) = -2\nabla_{XYZ} p_i$$

so that

(A.3.2)
$$\frac{1}{2}\nabla_{XYZ} \frac{\partial g_i^2}{\partial d_i} = -\boldsymbol{\Lambda}_i \ .$$

As pointed out in Section 3.2, the calculation of the corresponding derivatives with respect to φ_i and θ_i will be based on the matrices generated by the differential operator

$$\boldsymbol{\Gamma}_i = \nabla^T_{\xi_i \eta_i \varsigma_i}\left[\nabla_{XYZ}\right]$$

introduced in Section 3.2. In order to apply this operator to the individual errors $f_i^{\,2}$, g_i^2, we first apply the transposed gradient $\nabla^T_{\xi_i \eta_i \varsigma_i}$ to auxiliary quantities. In particular, note:

(A.3.3)

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{\Lambda}_i = \begin{bmatrix} \frac{\partial\xi_i}{\partial\xi_i} & \frac{\partial\xi_i}{\partial\eta_i} & \frac{\partial\xi_i}{\partial\varsigma_i} \\ \frac{\partial\eta_i}{\partial\xi_i} & \frac{\partial\eta_i}{\partial\eta_i} & \frac{\partial\eta_i}{\partial\varsigma_i} \\ \frac{\partial\varsigma_i}{\partial\xi_i} & \frac{\partial\varsigma_i}{\partial\eta_i} & \frac{\partial\varsigma_i}{\partial\varsigma_i} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \boldsymbol{I}\ ,\ \nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{U} = \begin{bmatrix} \frac{\partial X}{\partial\xi_i} & \frac{\partial X}{\partial\eta_i} & \frac{\partial X}{\partial\varsigma_i} \\ \frac{\partial Y}{\partial\xi_i} & \frac{\partial Y}{\partial\eta_i} & \frac{\partial Y}{\partial\varsigma_i} \\ \frac{\partial Z}{\partial\xi_i} & \frac{\partial Z}{\partial\eta_i} & \frac{\partial Z}{\partial\varsigma_i} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = \boldsymbol{0}$$

and

(A.3.4) $$\nabla^T_{\xi_i\eta_i\varsigma_i} p_i = \nabla^T_{\xi_i\eta_i\varsigma_i}(X\xi_i + Y\eta_i + Z\varsigma_i) = \begin{bmatrix} X & Y & Z \end{bmatrix} = \boldsymbol{U}^T\ ,$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} p_i^2 = 2p_i\nabla^T_{\xi_i\eta_i\varsigma_i}(p_i) = 2p_i\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} q_i^2 = \nabla^T_{\xi_i\eta_i\varsigma_i}(X^2 + Y^2 + Z^2 - p_i^2) = -\nabla^T_{\xi_i\eta_i\varsigma_i}(p_i^2) = -2p_i\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} q_i = \nabla^T_{\xi_i\eta_i\varsigma_i}\sqrt{q_i^2}) = \frac{1}{2}\frac{1}{\sqrt{q_i^2}}\nabla^T_{\xi_i\eta_i\varsigma_i}(q_i^2) = -\frac{p_i}{q_i}\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{q_i} = -\frac{1}{q_i^2}\nabla^T_{\xi_i\eta_i\varsigma_i}(q_i) = \frac{p_i}{q_i^3}\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} s_i^2 = \nabla^T_{\xi_i\eta_i\varsigma_i}(R^2 - q_i^2) = -\nabla^T_{\xi_i\eta_i\varsigma_i}(q_i^2) = 2p_i\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} s_i = \nabla^T_{\xi_i\eta_i\varsigma_i}\sqrt{s_i^2} = \frac{1}{2}\frac{1}{\sqrt{s_i^2}}\nabla^T_{\xi_i\eta_i\varsigma_i}(s_i^2) = \frac{p_i}{s_i}\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{s_i} = -\frac{1}{s_i^2}\nabla^T_{\xi_i\eta_i\varsigma_i}s_i) = -\frac{p_i}{s_i^3}\boldsymbol{U}^T$$

Consequently,

(A.3.5) $$\nabla^T_{\xi_i\eta_i\varsigma_i} f_i = \nabla^T_{\xi_i\eta_i\varsigma_i}(p_i - s_i - d_i) = \nabla^T_{\xi_i\eta_i\varsigma_i} p_i - \nabla^T_{\xi_i\eta_i\varsigma_i} s_i = \left(1 - \frac{p_i}{s_i}\right)\boldsymbol{U}^T = -\left(\frac{f_i + d_i}{s_i}\right)\boldsymbol{U}^T$$

With these intermediary results, we are able to determine the matrices $\boldsymbol{\Gamma}_i(f_i^2), \boldsymbol{\Gamma}_i(g_i^2)$. By (A.2.6) and the Product Rule,

$$\frac{1}{2}\boldsymbol{\Gamma}_i(f_i^2) = \nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{2}\nabla_{XYZ} f_i^2 = \nabla^T_{\xi_i\eta_i\varsigma_i}\left(\boldsymbol{U}\frac{f_i}{s_i} - \boldsymbol{\Lambda}_i\frac{f_i(f_i+d_i)}{s_i}\right)$$
$$= \boldsymbol{U}\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{f_i}{s_i}\right) - (\nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{\Lambda}_i)\frac{f_i(f_i+d_i)}{s_i} - \boldsymbol{\Lambda}_i\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{f_i(f_i+d_i)}{s_i}\right).$$

By (A.3.3-5),

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{f_i}{s_i}\right) = (\nabla^T_{\xi_i\eta_i\varsigma_i} f_i)\frac{1}{s_i} + f_i\nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{s_i} = -\left(\frac{f_i+d_i}{s_i}\right)\boldsymbol{U}^T\frac{1}{s_i} + f_i\left(-\frac{p_i}{s_i^3}\boldsymbol{U}^T\right)$$
$$= \left(-\frac{f_i+d_i}{s_i^2} - \frac{f_i p_i}{s_i^3}\right)\boldsymbol{U}^T = -\left(\frac{(f_i+d_i)s_i + f_i(f_i+s_i+d_i)}{s_i^3}\right)\boldsymbol{U}^T$$
$$= -\left(\frac{(f_i+d_i)s_i + f_i(f_i+d_i) + f_i s_i}{s_i^3}\right)\boldsymbol{U}^T = -\left(\frac{(f_i+d_i)(f_i+s_i) + f_i s_i}{s_i^3}\right)\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{f_i(f_i+d_i)}{s_i}\right) = \left(\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{f_i}{s_i}\right)\right)(f_i+d_i) + \frac{f_i}{s_i}\nabla^T_{\xi_i\eta_i\varsigma_i}(f_i+d_i)$$
$$= -\left(\left(\frac{(f_i+d_i)(f_i+s_i)+f_i s_i}{s_i^3}\right)(f_i+d_i) + \frac{f_i}{s_i}\left(\frac{f_i+d_i}{s_i}\right)\right)\boldsymbol{U}^T$$
$$= -\left(\frac{f_i+d_i}{s_i^3}\right)\big((f_i+d_i)(f_i+s_i) + f_i s_i + f_i s_i)\big)\boldsymbol{U}^T$$
$$= -\left(\frac{(f_i+d_i)\big((f_i+d_i)(f_i+s_i) + 2f_i s_i)\big)}{s_i^3}\right)\boldsymbol{U}^T$$

From this and by (A.3.3),
(A.3.6)
$$\frac{1}{2}\boldsymbol{\Gamma}_i(f_i^2) = -\left(\frac{(f_i+d_i)(f_i+s_i)+f_i s_i}{s_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T - \left(\frac{(f_i+d_i)\big((f_i+d_i)(f_i+s_i)+2f_i s_i)\big)}{s_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{U}^T$$
$$-\left(\frac{f_i(f_i+d_i)}{s_i}\right)\boldsymbol{I}$$

For the external portion g_i of the error function, we find similarly:

(A.3.7)
$$\frac{1}{2}\boldsymbol{\Gamma}_i(g_i^2) = \nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{2}\nabla_{XYZ}g_i^2 = \nabla^T_{\xi_i\eta_i\varsigma_i}\left(\boldsymbol{U}(1-\frac{R}{q_i}) + \boldsymbol{\Lambda}_i(\frac{Rp_i}{q_i}-d_i)\right)$$
$$= \boldsymbol{U}\nabla^T_{\xi_i\eta_i\varsigma_i}\left(-\frac{R}{q_i}\right) + (\nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{\Lambda}_i)(\frac{Rp_i}{q_i}-d_i) + \boldsymbol{\Lambda}_i\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{Rp_i}{q_i}\right).$$

By (A.3.4),

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\left(-\frac{R}{q_i}\right) = -\frac{Rp_i}{q_i^3}\boldsymbol{U}^T,$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{Rp_i}{q_i}\right) = \frac{R}{q_i}\left(\nabla^T_{\xi_i\eta_i\varsigma_i}p_i\right) + Rp_i\nabla^T_{\xi_i\eta_i\varsigma_i}\frac{1}{q_i}$$
$$= \left(\frac{R}{q_i} + \frac{Rp_i^2}{q_i^3}\right)\boldsymbol{U}^T = \left(\frac{R(q_i^2+p_i^2)}{q_i^3}\right)\boldsymbol{U}^T = \left(\frac{R(X^2+Y^2+Z^2)}{q_i^3}\right)\boldsymbol{U}^T$$

so that – in matrix notation--,

$$\frac{1}{2}\boldsymbol{\Gamma}_i(g_i^2) = \boldsymbol{U}\left(-\frac{Rp_i}{q_i^3}\right)\boldsymbol{U}^T + (\nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{\Lambda}_i)\left(\frac{Rp_i}{q_i}-d_i\right) + \boldsymbol{\Lambda}_i\left(\frac{R(X^2+Y^2+Z^2)}{q_i^3}\right)\boldsymbol{U}^T.$$

and finally,

(A.3.8)
$$\frac{1}{2}\boldsymbol{\Gamma}_i(g_i^2) = -\left(\frac{Rp_i}{q_i^3}\right)\boldsymbol{U}\boldsymbol{U}^T + \left(\frac{R(X^2+Y^2+Z^2)}{q_i^3}\right)\boldsymbol{\Lambda}_i\boldsymbol{U}^T + \left(\frac{Rp_i}{q_i}-d_i\right)\boldsymbol{I}.$$

A.4 Gradients and Hessians of the Orthogonal Error Function

We repeat the definitions of Chapter 4. The error function for orthogonal fitting of a sphere is given as

$$E_{orth} = \sum_{i=1}^{n}h_i^2 = \sum_{i=1}^{n}(w_i - R)^2 = w_i^2 - 2Rw_i + R^2$$

where

$$h_i = w_i - R$$

and

$$w_i^2 = (X - x_i)^2 + (Y - y_i)^2 + (Z - z_i)^2 = (X^2 + Y^2 + Z^2) - 2d_i p_i + d_i^2$$

with the notations (3.1.1)

$$x_i = d_i \cos\varphi_i \cos\theta_i = d_i\xi_i, \quad y_i = d_i \sin\varphi_i \cos\theta_i = d_i\eta_i, \quad z_i = d_i \sin\theta_i = d_i\xi_i,$$

and the definition (3.1.2) of the auxiliary quantity p_i. The vector
.

$$\boldsymbol{W}_i = \begin{bmatrix} X - x_i \\ Y - y_i \\ Z - z_i \end{bmatrix} = \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} - d_i \begin{bmatrix} \xi_i \\ \eta_i \\ \varsigma_i \end{bmatrix} = \boldsymbol{U} - d_i\boldsymbol{\Lambda}_i$$

will play the key role. Indeed, all the following gradients are multiples of $\boldsymbol{W}_i$:

(A.4.1) $$\nabla_{XYZ} w_i^2 = 2\boldsymbol{W}_i$$

$$\nabla_{XYZ} w_i = \nabla_{XYZ}\sqrt{w_i^2} = \frac{1}{2}\frac{1}{w_i}\nabla_{XYZ} w_i^2 = \frac{1}{w_i}\boldsymbol{W}_i ,$$

$$\nabla_{XYZ}\frac{1}{w_i} = -\frac{1}{w_i^2}\nabla_{XYZ} w_i = -\frac{1}{w_i^3}\boldsymbol{W}_i .$$

Thus

(A.4.2) $$\nabla_{XYZ} h_i = \nabla_{XYZ} w_i = \frac{1}{w_i}\boldsymbol{W}_i ,$$

and in view of

$$\nabla_{XYZ} h_i^2 = \nabla_{XYZ}(w_i - R)^2 = 2(w_i - R)\nabla_{XYZ} w_i = 2\frac{w_i - R}{w_i}\boldsymbol{W}_i ,$$

it follows that

(A.4.3) $$\frac{1}{2}\nabla_{XYZ} h_i^2 = \left(1 - \frac{R}{w_i}\right)\boldsymbol{W}_i \ .$$

Te Hessians of the quantities considered below are linear combinations of the two matrices

$$\boldsymbol{I} = \text{identity}, \qquad \text{and} \qquad \begin{bmatrix} X - x_i \\ Y - y_i \\ Z - z_i \end{bmatrix} \begin{bmatrix} X - x_i & Y - y_i & Z - z_i \end{bmatrix} = \boldsymbol{W}_i \boldsymbol{W}_i^T \cdot$$

In particular,

(A.4.4) $$\boldsymbol{H}_{XYZ} w_i^2 = \boldsymbol{H}_{XYZ}(X^2 + Y^2 + Z^2) - 2d_i \boldsymbol{H}_{XYZ} p_i + \boldsymbol{H}_{XYZ} d_i^2 = \boldsymbol{H}_{XYZ}(X^2 + Y^2 + Z^2) = 2\boldsymbol{I}$$

and by (A.1.2),

$$\begin{aligned} \boldsymbol{H}_{XYZ} w_i &= -\frac{1}{4}\frac{1}{w_i^3}\nabla_{XYZ} w_i^2 \nabla_{XYZ}^T w_i^2 + \frac{1}{2}\frac{1}{w_i}\boldsymbol{H}_{XYZ} w_i^2 = -\frac{1}{4}\frac{1}{w_i^3} 2\boldsymbol{W}_i\boldsymbol{W}_i^T 2 + \frac{1}{2}\frac{1}{w_i} 2\boldsymbol{I} \\ &= -\frac{1}{w_i^3}\boldsymbol{W}_i\boldsymbol{W}_i^T + \frac{1}{w_i}\boldsymbol{I}. \end{aligned}$$

As $h_i = w_i - R$ and $h_i^2 = w_i^2 - 2Rw_i + R^2$, we have

$$\boldsymbol{H}_{XYZ} h_i = \boldsymbol{H}_{XYZ} w_i = -\frac{1}{w_i^3}\boldsymbol{W}_i\boldsymbol{W}_i^T + \frac{1}{w_i}\boldsymbol{I} \ .$$

and

$$\boldsymbol{H}_{XYZ} h_i^2 = \boldsymbol{H}_{XYZ} w_i^2 - 2R\boldsymbol{H}_{XYZ} w_i = 2\boldsymbol{I} + \frac{2R}{w_i^3}\boldsymbol{W}_i\boldsymbol{W}_i^T - \frac{2R}{w_i}\boldsymbol{I} \ .$$

so that

(A.4.5) $$\frac{1}{2}\boldsymbol{H}_{XYZ} h_i^2 = \left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{R}{w_i^3}\boldsymbol{W}_i\boldsymbol{W}_i^T \ .$$

A.5 Mixed Derivatives of the Orthogonal Error Function

First, we differentiate with respect to the range variable d_i , starting with the key quantity w_i :

(A.5.1) $$\frac{\partial w_i^2}{\partial d_i} = \frac{\partial}{\partial d_i}(X^2 + Y^2 + Z^2 - 2d_i p_i + d_i^2) = -2(p_i - d_i)$$

$$\frac{\partial w_i}{\partial d_i} = \frac{1}{2}\frac{1}{w_i}\frac{\partial w_i^2}{\partial d_i} = \frac{1}{2}\frac{1}{w_i}(-2)(p_i - d_i) = -\frac{1}{w_i}(p_i - d_i)$$

$$\frac{\partial}{\partial d_i}\frac{1}{w_i} = -\frac{1}{w_i^2}\frac{\partial w}{\partial d_i} = -\frac{1}{w_i^3}(-1)(p_i - d_i) = \frac{1}{w_i^3}(p_i - d_i) \ .$$

Thus

$$\frac{\partial h_i^2}{\partial d_i} = \frac{\partial}{\partial d_i}(w_i - R)^2 = 2(w_i - R)\frac{\partial w_i}{\partial d_i} = -2\frac{w_i - R}{w_i}(p_i - d_i = -2\left(1 - \frac{R}{w_i}\right)(p_i - d_i)$$

and

$$\frac{1}{2}\nabla_{XYZ}\frac{\partial h_i^2}{\partial d_i} = -\left(-R\nabla_{XYZ}\frac{1}{w_i}\right)(p_i - d_i) - \left(1 - \frac{R}{w_i}\right)\nabla_{XYZ}\, p_i$$

so that, finally, by (A.4.1) and (3.2.1),

(A.5.2) $$\frac{1}{2}\nabla_{XYZ}\frac{\partial h_i^2}{\partial d_i} = -\frac{R}{w_i^3}(p_i - d_i)\boldsymbol{W}_i - \left(1 - \frac{R}{w_i}\right)\boldsymbol{\Lambda}_i \, .$$

We move to differentiation with respect to the bearing variables φ_i, θ_i. Again we aim to apply the differential matrix operator

$$\boldsymbol{\Gamma}_i = \nabla^T_{\xi_i\eta_i\varsigma_i}\left[\nabla_{XYZ}\right] ,$$

here to the individual orthogonal error h_i^2 -- expressed in matrix notation --:

$$\frac{1}{2}\boldsymbol{\Gamma}_i(h_i^2) = \nabla^T_{\xi_i\eta_i\varsigma_i}\left(\frac{1}{2}\nabla_{XYZ}h_i^2\right) = \nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{W}\left(1 - \frac{R}{w_i}\right) = (\nabla^T_{\xi_i\eta_i\varsigma_i}\boldsymbol{W})\left(1 - \frac{R}{w_i}\right) + \boldsymbol{W}\nabla^T_{\xi_i\eta_i\varsigma_i}\left(1 - \frac{R}{w_i}\right) .$$

By (A.3.3),

$$\nabla^T_{\xi_i\eta_i\varsigma_i} \boldsymbol{W}_i = -d_i \nabla^T_{\xi_i\eta_i\varsigma_i} \boldsymbol{\Lambda}_i = -d_i \boldsymbol{I} \ ,$$

and by (A.3.4),

$$\nabla^T_{\xi_i\eta_i\varsigma_i} w_{\mathrm{i}}^2 = \nabla^T_{\xi_i\eta_i\varsigma_i} \left((X^2 + Y^2 + Z^2) - 2d_i p_i + d_i^2 \right) = -2d_i \nabla^T_{\xi_i\eta_i\varsigma_i} p_i = -2d_i \boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} w_{\mathrm{i}} = \nabla^T_{\xi_i\eta_i\varsigma_i} \sqrt{w_{\mathrm{i}}^2} = \frac{1}{2}\frac{1}{\sqrt{w_{\mathrm{i}}^2}} \nabla^T_{\xi_i\eta_i\varsigma_i} w_{\mathrm{i}}^2 = -\frac{d_i}{w_i}\boldsymbol{U}^T$$

$$\nabla^T_{\xi_i\eta_i\varsigma_i} \frac{1}{w_{\mathrm{i}}} = -\frac{1}{w_{\mathrm{i}}} \nabla^T_{\xi_i\eta_i\varsigma_i} \mathrm{w}_{\mathrm{i}} = -\frac{1}{w_{\mathrm{i}}}\left(-\frac{d_i}{w_i}\boldsymbol{U}^T \right) = \frac{d_i}{w_i^3}\boldsymbol{U}^T$$

so that by (A.4.1),

$$\frac{1}{2}\boldsymbol{\Gamma}_i(h_i^2) = -d_i\left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{Rd_i}{w_i^3}\boldsymbol{W}\boldsymbol{U}^T \ .$$

Taking into account the orthogonality relations (3.2.10), this matrix can again be symmetrized by substituting $\boldsymbol{W}^T = \boldsymbol{U}^T + \boldsymbol{\Lambda}_i^T$ for $\boldsymbol{U}^T$ in the above expression, yielding the matrix

$$\frac{1}{2}\boldsymbol{\Gamma}_i^S(h_i^2) = -d_i\left(1 - \frac{R}{w_i}\right)\boldsymbol{I} + \frac{Rd_i}{w_i^3}\boldsymbol{W}\boldsymbol{W}^T \ .$$

Acknowledgement

We are grateful to our NIST colleagues James Filliben, Alan Heckert, and Joan Rosenblatt for discussions and material about the subject of variance propagation.

REFERENCES

[1] W. C. Stone, M. Juberts, N. Dagalakis, J. Stone, and J. Gorman, "Performance Analysis of Next-Generation LADAR for Manufacturing, Construction, and Mobility," *NISTIR* vol. 7117, 2004.

[2] D. E. Gilsinn, C. Witzgall, G. S. Cheok, and A. Lytle, "Construction Object Identification from LADAR Scans: An Experimental Study Using I-Beams," *NISTIR*, vol. 7286, 2005.

[3] P. J. Besl and N. D. McKay, "A method for registration of 3-D shapes," *IEEE Trans. Pattern Analysis and Machine Intelligence*, vol. 14, pp. 239-256, 1992.

[4] R. O. Duda and P. E. Hart, "Use of Hough transformation to detect lines and curve in pictures," *Comm. ACM*, vol. 15, pp. 11 - 15, 1972.

[5] K. Kanatani, *Statistical Optimization for Geometric Computation*. New York: Elsevier, 1996.

[6] A. C. Davidson, *Statistical Models*. Cambridge: Cambridge University Press, 2003.

[7] D. A. Freedman, *Statistical Models, Theory and Practice*, revised ed. Cambridge: Cambridge University Press, 2009.

[8] P. T. Boggs, J. R. Donaldson, R. B. Schnabel, and C. H. Spiegelman, "A computational examination of orthogonal distance regression," *Journal of Econometrics*, vol. 38, pp. 169 - 201, 1988.

[9] P. T. Boggs, J. R. Donaldson, R. H. Byrd, and R. B. Schnabel, "ALGORITHM 676 ODRPACK: Software for Weighted Orthogonal Distance Regression," *ACM Transactions on Mathematical Software*, vol. 15, pp. 348 - 364, 1989.

[10] W. Gander, G. H. Golub, and R. Strebel, "Least-squares fitting of circles and ellipses," *BIT*, vol. 34, pp. 558-578, 1994.

[11] C. M. Shakarji, "Least-Squares Fitting Algorithms of the NIST Algorithm Testing System," *Journal of Research of NIST*, vol. 103, pp. 633-640, 1998.

[12] S. J. Ahn, W. Rauh, and H. J. Warnecke, "Least-squares orthogonal distances fitting of circle, sphere, ellipse, hyperbola, and parabola," *Pattern Recognition*, vol. 34, pp. 2283-2303, 2001.

[13] I. D. Coope, "Circle Fitting by Linear and Nonlinear Least Squares," *J. Optimization Theory Applicat.*, vol. 76, pp. 381-388, 1993.

[14] B. A. Jones and R. B. Schnabel, "A comparison of two sphere fitting methods.," in *IEEE Proceedings of the Instrumentation and Measurement Technology*, 1986.

[15] I. Kasa, "A Circle Fitting Procedure and Its Error Analysis," *IEEE Trans. Instrum. Meas.*, vol. 25, pp. 8-14, 1976.

[16] Y. Nievergelt, "Computing circles and spheres of arithmetic least squares," *Comput. Phys. Commun.*, vol. 81, pp. 343-350, 1994.

[17] M. Renault, "Fitting Circles and Ellipses to Data Using the Least-Squares Method," in *http://www.math.temple.edu/~renault/ellipses.html*.

[18] H. Spath, "Least-Square Fitting with Spheres," *J. Optimization Theory Applicat.*, vol. 96, pp. 191-199, 1998.

[19] D. Umbach and K. N. Jones, "A Few Methods for Fitting Circles to Data," *IEEE Trans. Instrum. Meas.* , vol. 52, pp. 1881-1885, 2003.

[20] C. Witzgall, G. S. Cheok, and A. J. Kearsley, "Recovering Circles and Spheres from Point Data," in *Perspectives In Operations Research*, F. B. Alt, M. C. Fu, and B. L. Golden, Eds. New York: Springer, 2006, pp. 393-413.

[21] M. Franaszek, G. S. Cheok, K. S. Saidi, and C. Witzgall, "Fitting Spheres to Range Data from 3D Imaging Systems," *IEEE Trans. Instrum. Meas.* , 2009 - in print.

[22] M. Franaszek, G. S. Cheok, K. S. Saidi, and C. Witzgall, "Sphere Fitting as a Measure of 3D Imaging Systems Performance," in preparation, 2009.

[23] C. Witzgall and M. Franaszek, "Discussion of Variance Calculation for Linear and Nonlinear Regression," in preparation, 2009.

[24] GUM, "Evaluation of measurement data - Guide to the expression of uncertainty in measurement (http://www.bipm.org/en/publications/guides/gum.html)," JCGM 2008.
[25] H. Ku, "Notes on the Use of Propagation of Error Formulas," *Journal of Research National Bureau of Standards*, vol. 70C, pp. 331 - 341, 1966.
[26] D. M. Himmelblau, *Process Analysis by Statistical Methods*. New York: Wiley, 1970.
[27] N. R. Draper and H. Smith, *Applied Regression Analysis*, 2nd ed. New York: Wiley, 1981.
[28] C. G. Broyden, "The Convergence of a Class of Double-rank Minimization Algorithms: 2. The New Algorithm " *IMA J. Appl. Math.*, vol. 6, pp. 222 - 231, 1970.